Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
This journal is © The Royal Society of Chemistry 2017

Electronic Supplementary Information

Facile synthesis and electrochemistry of new cubic rocksalt $Li_xV_yO_2$ (x=0.78, y=0.75) electrode material

Wanqun Zhang,*[a] jingjing Luo,[b] xiaona Li,[b] Jianwen Liang,[b] Yongchun Zhu[b] and Yitai Qian[b]

[a] *School of Chemistry and Materials Science, University of Science and Technology of China, Hefei, 230026, P. R. China;* [b] *Division of Nanomaterials and chemistry, Hefei National Laboratory for Physical Sciences at MIcroscale, Department of Chemistry, University of Science and Technology of China, Hefei, 230026, Anhui, P. R.China.*

* *To whom correspondence should be addressed. E-mail: wqz@ustc.edu.cn.*

Table S1. Crystallographic parameters for as-prepared $Li_{0.78}V_{0.75}O_2$.

$Fm\bar{3}m$. a = 4.3247(12)

Atom	Wyckoff symbol	x/a	y/b	z/c	Biso	occupancy
Li	4a	0	0	0	2.69(6)	0.391(6)
V	4a	0	0	0	2.69(6)	0.375(4)
O	4b	0.5	0.5	0.5	1.85(4)	1

R-factors: R_{exp} = 6.02%, R_{wp} = 6.16%, R_p =4.70%

Table S2. Crystallographic parameters for $Li_xV_yO_2$ obtained by annealing $Li_{0.78}V_{0.75}O_2$ at 800 ℃ in argon.

$R\bar{3}m$. a = 2.9659(7), c=14.910(3)

Atom	Wyckoff symbol	x/a	y/b	z/c	Biso	occupancy
Li	3a	0	0	0	3.1(3)	0.83(5)
V	3b	0	0	0.5	1.05(3)	0.77(3)
O	6c	0	0	0.24617(14)	2.144(5)	1

R-factors: R_{exp} = 4.25%, R_{wp} = 8.63%, R_p = 6.16%

Table. S3. Comparison of $Li_{0.78}V_{0.75}O_2$ (this work) and various reported $Li_xV_yO_2$ composites as anodes for Li-ion batteries.

Material	**Reversible capacity/mAh g^{-1}**	**Rate**	**Ref**
$Li_{0.78}V_{0.75}O_2$	500/500th cycles	500 mA g^{-1}	This work
$Li_{1+0.2}VO_2$	294/25th cycles	0.1 C	12
$Li_{1.07}V_{0.93}O_2$	100/10th cycles	10 mA g^{-1}	22
Carbon-coat $Li_{1.1}V_{0.9}O_2$	150/20th cycles	0.1 C	28
$Li_{1.075}V_{0.925}O_2$	～175/30th cycles	44 mA g^{-1}	29

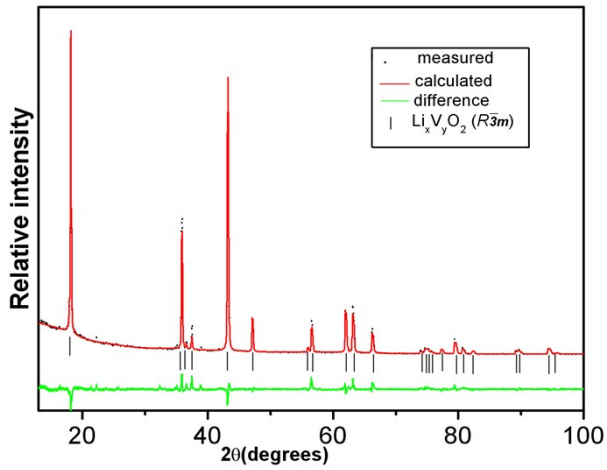

Fig. S1 Refined powder X-ray diffraction pattern for $Li_xV_yO_2$ obtained by annealing $Li_{0.78}V_{0.75}O_2$ at 800 ℃ in a following argon atmosphere. Dots represent observed data and solid line the calculated pattern. The lower line is the difference/esd.

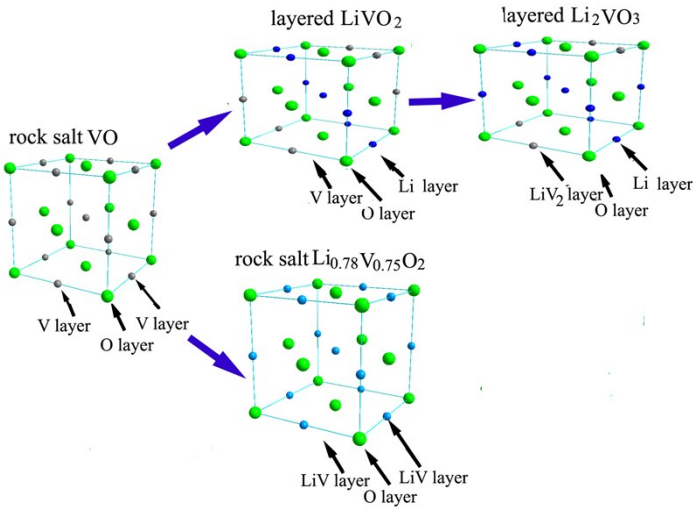

Fig. S2 Structural illustration of rock salt VO and $Li_{0.78}V_{0.75}O_2$， layered $LiVO_2$ and Li_2VO_3

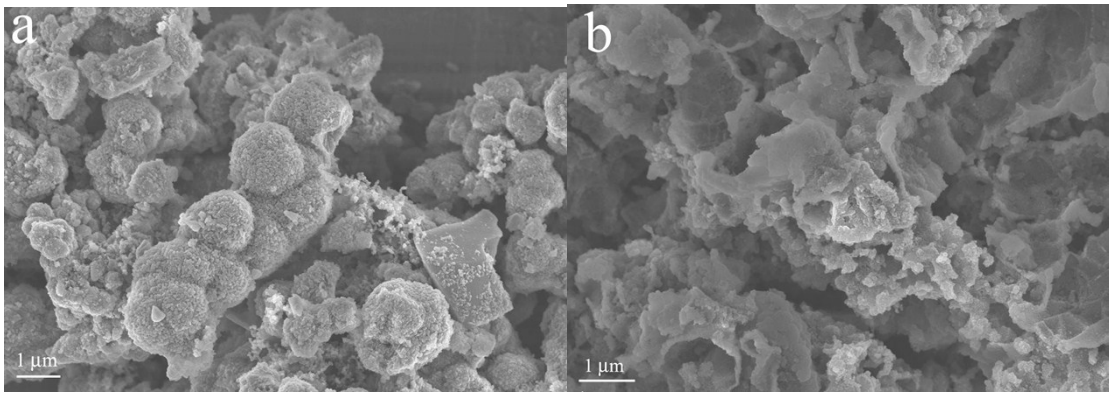

Fig. S3 FESEM images of $Li_{0.78}V_{0.75}O_2$ composite electrode after 40 (a) and 150 (b) electrochemical cycles at the current of 500 mA g^{-1}, respectively